



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 06:18 AM UTC

PDB ID : 3UNW / pdb_00003unw
Title : Crystal Structure of Human GAC in Complex with Glutamate
Authors : DeLaBarre, B.; Gross, S.; Cheng, F.; Gao, Y.; Jha, A.; Jiang, F.; Song, J.J.;
Wie, W.; Hurov, J.
Deposited on : 2011-11-16
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

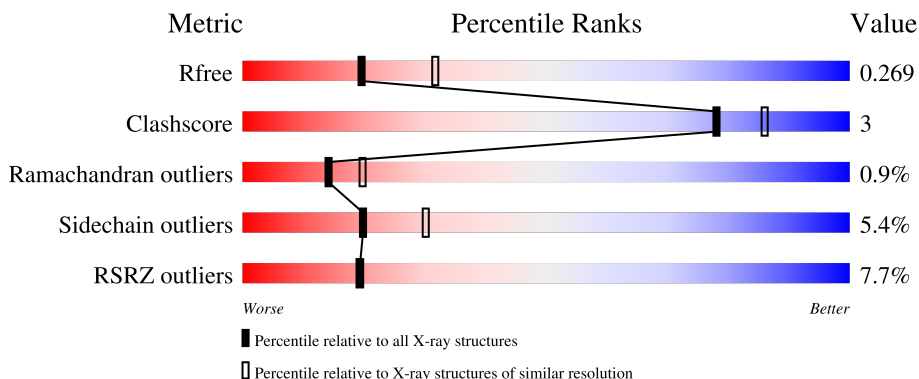
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	 6% 62% 13% 24%
1	B	534	 6% 62% 10% 25%
1	C	534	 5% 63% 11% 25%
1	D	534	 6% 60% 13% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12769 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	9	0	0
			3162	2014	532	588	28			
1	B	400	Total	C	N	O	S	6	0	0
			3123	1993	525	577	28			
1	C	400	Total	C	N	O	S	25	0	0
			3124	1995	525	576	28			
1	D	403	Total	C	N	O	S	13	0	0
			3141	2001	528	584	28			

There are 24 discrepancies between the modelled and reference sequences:

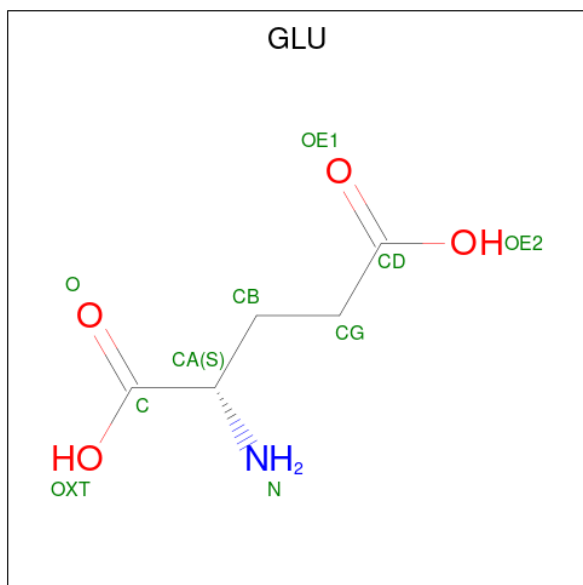
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	HIS	-	expression tag	UNP O94925
A	600	HIS	-	expression tag	UNP O94925
A	601	HIS	-	expression tag	UNP O94925
A	602	HIS	-	expression tag	UNP O94925
A	603	HIS	-	expression tag	UNP O94925
A	604	HIS	-	expression tag	UNP O94925
B	599	HIS	-	expression tag	UNP O94925
B	600	HIS	-	expression tag	UNP O94925
B	601	HIS	-	expression tag	UNP O94925
B	602	HIS	-	expression tag	UNP O94925
B	603	HIS	-	expression tag	UNP O94925
B	604	HIS	-	expression tag	UNP O94925
C	599	HIS	-	expression tag	UNP O94925
C	600	HIS	-	expression tag	UNP O94925
C	601	HIS	-	expression tag	UNP O94925
C	602	HIS	-	expression tag	UNP O94925
C	603	HIS	-	expression tag	UNP O94925
C	604	HIS	-	expression tag	UNP O94925
D	599	HIS	-	expression tag	UNP O94925
D	600	HIS	-	expression tag	UNP O94925
D	601	HIS	-	expression tag	UNP O94925

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Chain	Residue	Modelled	Actual	Comment	Reference
D	602	HIS	-	expression tag	UNP O94925
D	603	HIS	-	expression tag	UNP O94925
D	604	HIS	-	expression tag	UNP O94925

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).

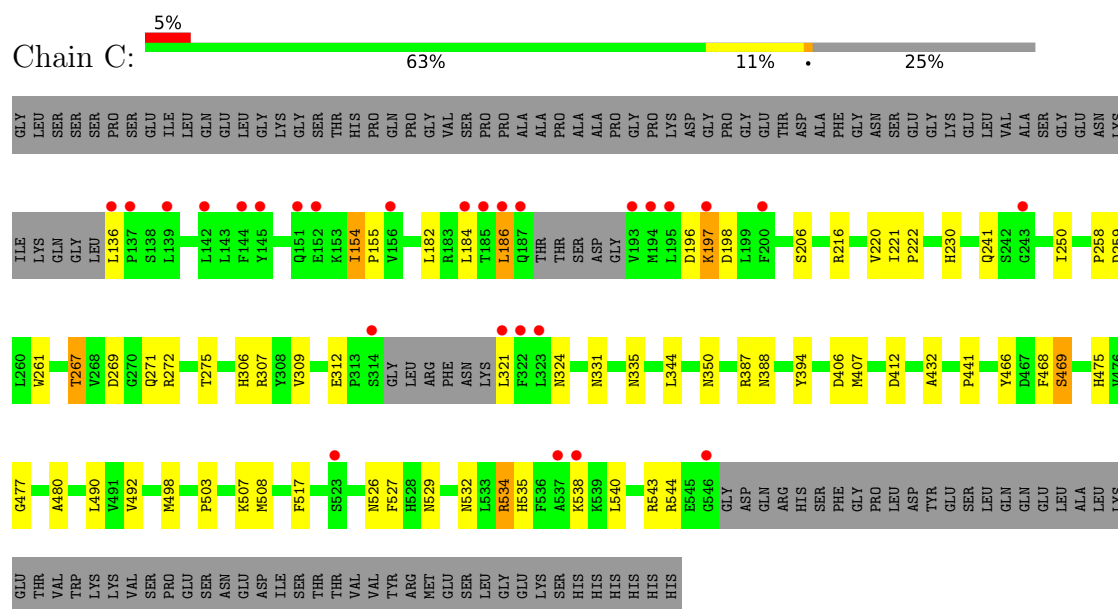


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		

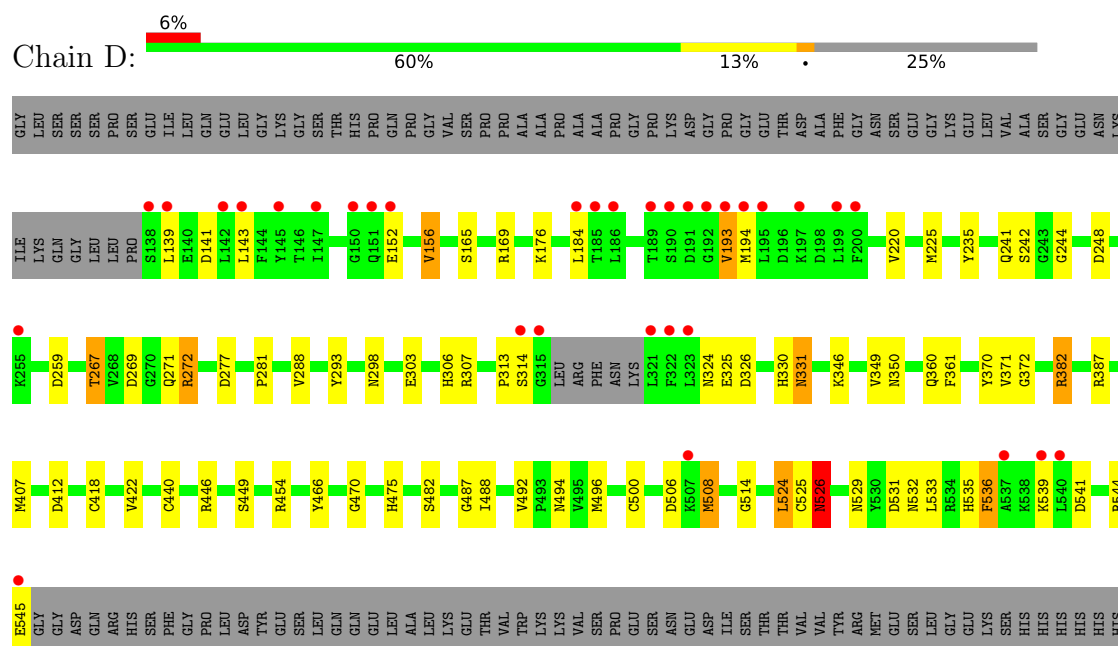
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	43	Total	O	0	0
			43	43		
3	C	46	Total	O	0	0
			46	46		
3	D	44	Total	O	0	0
			44	44		

• Molecule 1: Glutaminase kidney isoform, mitochondrial



• Molecule 1: Glutaminase kidney isoform, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.66Å 139.61Å 178.38Å 90.00° 94.14° 90.00°	Depositor
Resolution (Å)	29.04 – 2.56 29.04 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.04-2.56) 99.7 (29.04-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.261 0.232 , 0.269	Depositor DCC
R_{free} test set	4013 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12769	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.45	5/3232 (0.2%)	1.45	27/4364 (0.6%)
1	B	1.46	6/3192 (0.2%)	1.45	32/4307 (0.7%)
1	C	1.44	5/3193 (0.2%)	1.40	21/4309 (0.5%)
1	D	1.45	7/3210 (0.2%)	1.44	30/4333 (0.7%)
All	All	1.45	23/12827 (0.2%)	1.44	110/17313 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	10
1	C	0	5
1	D	0	12
All	All	0	34

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	372	GLY	CA-C	-7.10	1.46	1.52
1	B	483	GLY	N-CA	-6.77	1.38	1.45
1	B	501	TRP	NE1-CE2	-6.10	1.30	1.37
1	C	230	HIS	CB-CG	-5.85	1.42	1.50
1	A	541	ASP	N-CA	-5.71	1.41	1.46
1	A	538	LYS	CA-C	-5.69	1.46	1.53
1	D	525	CYS	C-N	-5.61	1.25	1.33
1	B	497	GLY	CA-C	-5.43	1.46	1.52
1	D	487	GLY	CA-C	-5.41	1.46	1.52
1	B	262	GLY	CA-C	-5.40	1.47	1.51
1	C	475	HIS	CB-CG	-5.36	1.42	1.50
1	D	500	CYS	CA-C	-5.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	539	LYS	N-CA	-5.34	1.39	1.46
1	D	244	GLY	CA-C	-5.29	1.46	1.52
1	C	503	PRO	CA-CB	-5.28	1.46	1.54
1	D	475	HIS	CE1-NE2	-5.27	1.27	1.32
1	C	477	GLY	CA-C	-5.26	1.46	1.51
1	D	470	GLY	CA-C	-5.26	1.46	1.52
1	A	261	TRP	NE1-CE2	-5.17	1.31	1.37
1	B	306	HIS	CE1-NE2	-5.15	1.27	1.32
1	A	262	GLY	CA-C	-5.04	1.46	1.51
1	C	309	VAL	C-O	-5.03	1.19	1.24
1	B	503	PRO	CA-CB	-5.00	1.47	1.54

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	526	ASN	CA-CB-CG	12.43	125.03	112.60
1	B	306	HIS	CA-CB-CG	-8.30	105.50	113.80
1	B	259	ASP	CA-CB-CG	-7.90	104.70	112.60
1	D	496	MET	CA-C-N	7.76	127.53	122.18
1	D	496	MET	C-N-CA	7.76	127.53	122.18
1	B	324	ASN	CA-CB-CG	7.68	120.28	112.60
1	A	259	ASP	CA-CB-CG	-7.67	104.93	112.60
1	C	306	HIS	CA-CB-CG	-7.64	106.16	113.80
1	C	324	ASN	CA-CB-CG	7.60	120.20	112.60
1	D	506	ASP	CA-CB-CG	7.56	120.16	112.60
1	D	324	ASN	CA-CB-CG	7.52	120.12	112.60
1	D	541	ASP	CA-C-N	7.31	127.95	119.47
1	D	541	ASP	C-N-CA	7.31	127.95	119.47
1	A	277	ASP	CA-CB-CG	-7.26	105.33	112.60
1	D	248	ASP	CA-CB-CG	7.21	119.81	112.60
1	B	535	HIS	CA-CB-CG	7.09	120.89	113.80
1	A	154	ILE	O-C-N	-6.99	116.96	121.37
1	C	312	GLU	O-C-N	-6.97	117.25	121.71
1	A	541	ASP	CA-C-N	6.67	126.92	119.32
1	A	541	ASP	C-N-CA	6.67	126.92	119.32
1	D	306	HIS	CA-CB-CG	-6.62	107.18	113.80
1	D	331	ASN	CA-C-N	6.62	126.56	119.28
1	D	331	ASN	C-N-CA	6.62	126.56	119.28
1	B	194	MET	CG-SD-CE	-6.57	86.44	100.90
1	A	194	MET	CG-SD-CE	-6.53	86.55	100.90
1	B	532	ASN	CA-CB-CG	-6.45	106.15	112.60
1	D	492	VAL	CA-C-N	6.40	126.78	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	492	VAL	C-N-CA	6.40	126.78	119.93
1	D	350	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	527	PHE	CA-CB-CG	-6.35	107.45	113.80
1	D	482	SER	CA-C-N	6.31	127.01	121.58
1	D	482	SER	C-N-CA	6.31	127.01	121.58
1	B	531	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	527	PHE	N-CA-C	6.26	124.13	110.80
1	C	406	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	331	ASN	CA-C-N	6.14	125.83	119.56
1	C	331	ASN	C-N-CA	6.14	125.83	119.56
1	B	248	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	344	LEU	N-CA-C	6.01	118.62	111.71
1	D	194	MET	CG-SD-CE	-5.98	87.74	100.90
1	D	360	GLN	CB-CG-CD	-5.95	102.48	112.60
1	C	534	ARG	N-CA-C	5.94	117.55	111.14
1	D	544	ARG	N-CA-C	5.91	117.52	111.14
1	C	221	ILE	O-C-N	-5.80	116.93	121.46
1	A	306	HIS	CA-CB-CG	-5.80	108.00	113.80
1	A	482	SER	CA-C-N	5.77	127.29	121.35
1	A	482	SER	C-N-CA	5.77	127.29	121.35
1	C	469	SER	CA-C-N	5.74	126.20	119.94
1	C	469	SER	C-N-CA	5.74	126.20	119.94
1	A	496	MET	CA-C-N	5.72	126.13	122.18
1	A	496	MET	C-N-CA	5.72	126.13	122.18
1	B	503	PRO	O-C-N	-5.71	114.72	121.46
1	B	250	ILE	CA-C-N	5.70	125.81	119.32
1	B	250	ILE	C-N-CA	5.70	125.81	119.32
1	B	469	SER	CA-C-N	5.67	126.24	120.00
1	B	469	SER	C-N-CA	5.67	126.24	120.00
1	A	475	HIS	CA-CB-CG	-5.66	108.14	113.80
1	A	506	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	312	GLU	CA-C-N	5.59	125.54	119.78
1	B	312	GLU	C-N-CA	5.59	125.54	119.78
1	C	198	ASP	CA-CB-CG	-5.58	107.02	112.60
1	D	371	VAL	CA-C-N	5.56	126.49	121.82
1	D	371	VAL	C-N-CA	5.56	126.49	121.82
1	B	407	MET	CG-SD-CE	-5.56	88.67	100.90
1	B	344	LEU	N-CA-C	5.55	118.09	111.71
1	A	527	PHE	N-CA-C	5.52	118.06	111.71
1	B	449	SER	CA-C-N	5.48	125.14	119.05
1	B	449	SER	C-N-CA	5.48	125.14	119.05
1	D	313	PRO	CB-CA-C	5.45	118.56	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	355	PHE	CA-CB-CG	-5.42	108.38	113.80
1	B	272	ARG	CB-CG-CD	5.42	123.77	111.30
1	D	524	LEU	N-CA-C	5.41	116.86	111.07
1	D	440	CYS	O-C-N	-5.38	116.18	121.18
1	A	172	ASP	CA-C-N	5.37	125.44	119.32
1	A	172	ASP	C-N-CA	5.37	125.44	119.32
1	A	331	ASN	CA-C-N	5.32	125.14	119.28
1	A	331	ASN	C-N-CA	5.32	125.14	119.28
1	B	536	PHE	CA-C-N	-5.30	114.34	121.71
1	B	536	PHE	C-N-CA	-5.30	114.34	121.71
1	C	350	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	350	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	250	ILE	CA-C-N	5.26	125.32	119.32
1	C	250	ILE	C-N-CA	5.26	125.32	119.32
1	C	527	PHE	N-CA-C	5.26	117.76	111.71
1	D	508	MET	CG-SD-CE	-5.26	89.33	100.90
1	B	443	THR	N-CA-C	5.25	117.92	111.82
1	C	492	VAL	CB-CA-C	-5.25	106.09	111.08
1	A	309	VAL	CA-C-N	5.23	127.23	120.64
1	A	309	VAL	C-N-CA	5.23	127.23	120.64
1	D	176	LYS	N-CA-C	5.20	116.63	111.07
1	A	312	GLU	O-C-N	-5.20	118.21	121.85
1	C	261	TRP	CA-CB-CG	5.19	123.47	113.60
1	A	455	ASN	CA-CB-CG	5.16	117.76	112.60
1	C	196	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	154	ILE	O-C-N	-5.09	116.83	121.41
1	A	280	VAL	N-CA-C	5.09	113.01	108.63
1	C	503	PRO	O-C-N	-5.09	115.45	121.46
1	B	313	PRO	CB-CA-C	5.08	117.73	111.23
1	D	382	ARG	CA-CB-CG	5.08	124.26	114.10
1	B	154	ILE	O-C-N	-5.08	117.50	121.46
1	B	496	MET	CA-C-N	5.06	127.62	122.66
1	B	496	MET	C-N-CA	5.06	127.62	122.66
1	B	172	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	331	ASN	CA-C-N	5.01	125.08	119.87
1	B	331	ASN	C-N-CA	5.01	125.08	119.87
1	A	360	GLN	CB-CG-CD	-5.00	104.09	112.60
1	D	545	GLU	N-CA-CB	5.00	119.01	110.50
1	B	503	PRO	N-CA-C	5.00	116.81	110.70
1	D	244	GLY	CA-C-O	-5.00	118.85	122.45

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ARG	Sidechain
1	A	235	TYR	Sidechain
1	A	272	ARG	Sidechain
1	A	382	ARG	Sidechain
1	A	466	TYR	Sidechain
1	A	534	ARG	Sidechain
1	A	536	PHE	Mainchain
1	B	145	TYR	Sidechain
1	B	216	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	235	TYR	Sidechain
1	B	293	TYR	Sidechain
1	B	382	ARG	Sidechain
1	B	454	ARG	Sidechain
1	B	466	TYR	Sidechain
1	B	535	HIS	Mainchain
1	B	543	ARG	Sidechain
1	C	272	ARG	Sidechain
1	C	394	TYR	Sidechain
1	C	466	TYR	Sidechain
1	C	534	ARG	Sidechain
1	C	544	ARG	Sidechain
1	D	169	ARG	Sidechain
1	D	235	TYR	Sidechain
1	D	272	ARG	Sidechain
1	D	293	TYR	Sidechain
1	D	370	TYR	Sidechain
1	D	382	ARG	Sidechain
1	D	446	ARG	Sidechain
1	D	454	ARG	Sidechain
1	D	466	TYR	Sidechain
1	D	524	LEU	Mainchain
1	D	526	ASN	Mainchain
1	D	536	PHE	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3162	0	3126	18	6
1	B	3123	0	3100	20	1
1	C	3124	0	3103	17	8
1	D	3141	0	3112	19	3
2	A	10	0	5	0	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	D	10	0	5	1	0
3	A	46	0	0	0	0
3	B	43	0	0	0	0
3	C	46	0	0	0	0
3	D	44	0	0	0	1
All	All	12769	0	12461	69	12

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASN:HD22	1:A:535:HIS:H	1.18	0.91
1:C:532:ASN:HD22	1:C:535:HIS:H	1.24	0.85
1:A:267:THR:HG22	1:A:269:ASP:H	1.43	0.81
1:D:267:THR:HG22	1:D:269:ASP:H	1.46	0.80
1:B:267:THR:HG22	1:B:269:ASP:H	1.50	0.77
1:B:267:THR:HG21	1:B:271:GLN:OE1	1.95	0.66
1:B:272:ARG:HG2	1:B:272:ARG:HH11	1.61	0.64
1:D:298:ASN:HD22	1:D:449:SER:H	1.50	0.60
1:C:267:THR:HG22	1:C:269:ASP:H	1.67	0.59
1:D:156:VAL:HB	1:D:193:VAL:HG22	1.84	0.59
1:A:529:ASN:HD21	1:C:529:ASN:HD21	1.50	0.59
1:B:216:ARG:HH11	1:B:216:ARG:HA	1.67	0.59
1:D:532:ASN:HD22	1:D:535:HIS:H	1.49	0.58
1:A:267:THR:HG22	1:A:269:ASP:N	2.20	0.53
1:B:494:ASN:ND2	1:D:533:LEU:H	2.07	0.53
1:B:267:THR:HG22	1:B:269:ASP:N	2.23	0.52
1:B:498:MET:HE1	1:B:517:PHE:CE2	2.44	0.52
1:C:197:LYS:C	1:C:197:LYS:HD2	2.36	0.51
1:A:267:THR:HG21	1:A:271:GLN:OE1	2.11	0.50
1:B:498:MET:HE1	1:B:517:PHE:HE2	1.76	0.50
1:D:418:CYS:HG	2:D:800:GLU:N	2.10	0.50
1:A:498:MET:HE1	1:A:517:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:THR:HG22	1:D:269:ASP:N	2.22	0.49
1:C:267:THR:HG21	1:C:271:GLN:OE1	2.13	0.48
1:D:267:THR:CG2	1:D:269:ASP:H	2.21	0.48
1:B:267:THR:CG2	1:B:269:ASP:H	2.23	0.48
1:D:532:ASN:HD22	1:D:535:HIS:N	2.10	0.48
1:D:267:THR:HG21	1:D:271:GLN:OE1	2.13	0.48
1:C:532:ASN:ND2	1:C:535:HIS:H	2.03	0.47
1:B:533:LEU:H	1:D:494:ASN:ND2	2.12	0.47
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.79	0.47
1:C:468:PHE:HD1	1:C:508:MET:HE3	1.80	0.47
1:B:220:VAL:CG1	1:B:267:THR:HG23	2.45	0.47
1:D:526:ASN:HA	1:D:531:ASP:OD2	2.14	0.47
1:D:165:SER:HB2	1:D:225:MET:SD	2.55	0.47
1:D:281:PRO:HA	1:D:422:VAL:O	2.16	0.46
1:A:220:VAL:CG1	1:A:267:THR:HG23	2.46	0.46
1:C:220:VAL:CG1	1:C:267:THR:HG23	2.46	0.46
1:C:267:THR:HG22	1:C:269:ASP:N	2.29	0.45
1:C:154:ILE:HG22	1:C:155:PRO:O	2.16	0.45
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.99	0.45
1:D:220:VAL:CG1	1:D:267:THR:HG23	2.47	0.44
1:A:529:ASN:HD21	1:C:529:ASN:ND2	2.14	0.44
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.99	0.44
1:A:410:ILE:HD13	1:A:410:ILE:HA	1.90	0.43
1:C:480:ALA:HB2	1:C:490:LEU:HD12	2.00	0.43
1:B:216:ARG:O	1:B:217:ARG:HB2	2.18	0.43
1:B:343:SER:HA	1:B:410:ILE:HD12	2.00	0.43
1:B:536:PHE:CD2	1:B:536:PHE:N	2.83	0.43
1:B:538:LYS:O	1:B:539:LYS:HG3	2.18	0.43
1:A:227:PHE:CZ	1:A:231:ILE:HD11	2.54	0.42
1:C:432:ALA:HB1	1:C:441:PRO:HG3	2.01	0.42
1:B:235:TYR:CE1	1:B:261:TRP:CD1	3.07	0.42
1:A:486:GLY:HA3	1:A:502:SER:O	2.20	0.42
1:B:248:ASP:HA	1:B:254:ALA:HB2	2.00	0.42
1:C:182:LEU:O	1:C:186:LEU:HB2	2.19	0.42
1:A:248:ASP:HA	1:A:254:ALA:HB2	2.02	0.42
1:A:272:ARG:HH11	1:A:272:ARG:HG2	1.85	0.41
1:C:335:ASN:HD22	1:C:388:ASN:HD21	1.68	0.41
1:A:407:MET:HE3	1:A:408:VAL:HG22	2.03	0.41
1:B:532:ASN:HA	1:D:494:ASN:HD21	1.85	0.41
1:C:517:PHE:CD2	1:C:517:PHE:C	2.99	0.41
1:D:314:SER:HB3	1:D:330:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:MET:HE1	1:C:517:PHE:HE2	1.85	0.40
1:D:330:HIS:O	1:D:331:ASN:HB3	2.21	0.40
1:D:488:ILE:HD12	1:D:514:GLY:HA3	2.03	0.40
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.87	0.40
1:A:527:PHE:CZ	1:A:542:PRO:HG2	2.56	0.40
1:A:541:ASP:HA	1:A:542:PRO:HD2	1.84	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:CD	1:C:538:LYS:NZ[1_455]	0.60	1.60
1:A:236:GLU:OE1	1:C:538:LYS:NZ[1_455]	0.69	1.51
1:C:259:ASP:OD1	1:C:307:ARG:NH2[1_655]	1.32	0.88
1:D:259:ASP:OD1	1:D:307:ARG:NH2[1_455]	1.44	0.76
1:A:236:GLU:OE1	1:C:538:LYS:CE[1_455]	1.54	0.66
1:A:236:GLU:OE2	1:C:538:LYS:NZ[1_455]	1.55	0.65
1:A:236:GLU:CD	1:C:538:LYS:CE[1_455]	1.92	0.28
1:A:236:GLU:CG	1:C:538:LYS:NZ[1_455]	1.98	0.22
1:D:259:ASP:CG	1:D:307:ARG:NH2[1_455]	2.07	0.13
1:C:259:ASP:CG	1:C:307:ARG:NH2[1_655]	2.12	0.08
1:D:242:SER:CB	1:D:303:GLU:OE2[1_455]	2.17	0.03
1:B:198:ASP:OD2	3:D:70:HOH:O[2_556]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/534 (76%)	384 (95%)	17 (4%)	2 (0%)	24	33
1	B	394/534 (74%)	373 (95%)	16 (4%)	5 (1%)	9	12
1	C	394/534 (74%)	374 (95%)	15 (4%)	5 (1%)	9	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	399/534 (75%)	383 (96%)	14 (4%)	2 (0%)	24	33
All	All	1590/2136 (74%)	1514 (95%)	62 (4%)	14 (1%)	14	20

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	VAL
1	B	217	ARG
1	B	322	PHE
1	B	527	PHE
1	D	193	VAL
1	A	192	GLY
1	C	241	GLN
1	C	469	SER
1	B	539	LYS
1	B	287	CYS
1	C	222	PRO
1	C	186	LEU
1	D	241	GLN
1	C	526	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/458 (76%)	328 (94%)	22 (6%)	16	23
1	B	347/458 (76%)	330 (95%)	17 (5%)	22	33
1	C	347/458 (76%)	332 (96%)	15 (4%)	26	38
1	D	349/458 (76%)	327 (94%)	22 (6%)	16	23
All	All	1393/1832 (76%)	1317 (94%)	76 (6%)	20	29

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LEU
1	A	143	LEU
1	A	156	VAL
1	A	184	LEU
1	A	195	LEU
1	A	198	ASP
1	A	216	ARG
1	A	258	PRO
1	A	267	THR
1	A	272	ARG
1	A	275	THR
1	A	288	VAL
1	A	322	PHE
1	A	325	GLU
1	A	353	GLU
1	A	361	PHE
1	A	387	ARG
1	A	407	MET
1	A	412	ASP
1	A	450	PRO
1	A	520	ASP
1	A	545	GLU
1	B	139	LEU
1	B	152	GLU
1	B	186	LEU
1	B	201	LYS
1	B	216	ARG
1	B	267	THR
1	B	275	THR
1	B	288	VAL
1	B	325	GLU
1	B	353	GLU
1	B	387	ARG
1	B	407	MET
1	B	412	ASP
1	B	450	PRO
1	B	520	ASP
1	B	536	PHE
1	B	538	LYS
1	C	136	LEU
1	C	184	LEU
1	C	197	LYS
1	C	206	SER

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Mol	Chain	Res	Type
1	C	216	ARG
1	C	258	PRO
1	C	267	THR
1	C	275	THR
1	C	321	LEU
1	C	387	ARG
1	C	407	MET
1	C	412	ASP
1	C	507	LYS
1	C	540	LEU
1	C	543	ARG
1	D	139	LEU
1	D	141	ASP
1	D	143	LEU
1	D	152	GLU
1	D	156	VAL
1	D	184	LEU
1	D	267	THR
1	D	272	ARG
1	D	288	VAL
1	D	325	GLU
1	D	326	ASP
1	D	346	LYS
1	D	349	VAL
1	D	361	PHE
1	D	387	ARG
1	D	407	MET
1	D	412	ASP
1	D	508	MET
1	D	526	ASN
1	D	529	ASN
1	D	536	PHE
1	D	539	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	A	471	GLN
1	A	516	HIS
1	A	529	ASN
1	A	532	ASN

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Mol	Chain	Res	Type
1	A	535	HIS
1	B	388	ASN
1	B	471	GLN
1	B	494	ASN
1	B	529	ASN
1	C	205	GLN
1	C	330	HIS
1	C	375	ASN
1	C	388	ASN
1	C	471	GLN
1	C	510	ASN
1	C	529	ASN
1	C	532	ASN
1	D	157	HIS
1	D	298	ASN
1	D	330	HIS
1	D	375	ASN
1	D	379	GLN
1	D	388	ASN
1	D	471	GLN
1	D	494	ASN
1	D	510	ASN
1	D	519	HIS
1	D	532	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLU	D	800	-	8,9,9	1.10	1 (12%)	8,11,11	0.85	0
2	GLU	A	800	-	8,9,9	1.19	1 (12%)	8,11,11	1.46	1 (12%)
2	GLU	C	800	-	8,9,9	1.06	1 (12%)	8,11,11	1.27	1 (12%)
2	GLU	B	800	-	8,9,9	1.13	1 (12%)	8,11,11	1.53	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	D	800	-	-	4/9/9/9	-
2	GLU	A	800	-	-	3/9/9/9	-
2	GLU	C	800	-	-	0/9/9/9	-
2	GLU	B	800	-	-	2/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	GLU	OE2-CD	-2.09	1.23	1.30
2	C	800	GLU	OE2-CD	-2.08	1.23	1.30
2	A	800	GLU	OXT-C	-2.06	1.24	1.30
2	B	800	GLU	OE2-CD	-2.05	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	GLU	CB-CA-C	-3.33	101.62	110.45
2	B	800	GLU	CB-CA-C	-2.88	102.83	110.45
2	C	800	GLU	CB-CA-C	-2.65	103.44	110.45

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	800	GLU	N-CA-CB-CG
2	D	800	GLU	OE1-CD-CG-CB
2	D	800	GLU	OE2-CD-CG-CB
2	A	800	GLU	OE2-CD-CG-CB
2	B	800	GLU	OE2-CD-CG-CB
2	A	800	GLU	OE1-CD-CG-CB
2	B	800	GLU	OE1-CD-CG-CB
2	D	800	GLU	C-CA-CB-CG
2	A	800	GLU	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	800	GLU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	407/534 (76%)	0.55	30 (7%)	20 20	24, 39, 80, 96	2 (0%)
1	B	400/534 (74%)	0.54	34 (8%)	16 16	24, 39, 78, 89	1 (0%)
1	C	400/534 (74%)	0.56	27 (6%)	23 23	24, 39, 78, 92	6 (1%)
1	D	403/534 (75%)	0.55	33 (8%)	17 17	24, 39, 78, 89	3 (0%)
All	All	1610/2136 (75%)	0.55	124 (7%)	19 19	24, 39, 78, 96	12 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	321	LEU	8.4
1	C	136	LEU	7.3
1	C	193	VAL	5.9
1	A	321	LEU	5.7
1	C	322	PHE	5.6
1	B	193	VAL	5.3
1	B	322	PHE	5.2
1	B	137	PRO	5.1
1	D	322	PHE	5.0
1	B	152	GLU	5.0
1	D	315	GLY	4.7
1	C	321	LEU	4.6
1	A	322	PHE	4.3
1	B	195	LEU	4.2
1	B	188	THR	4.2
1	A	193	VAL	4.2
1	D	193	VAL	4.1
1	A	135	LEU	4.1
1	D	537	ALA	4.0
1	A	191	ASP	4.0
1	C	537	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	190	SER	3.9
1	B	149	GLU	3.8
1	C	546	GLY	3.7
1	D	197	LYS	3.7
1	C	152	GLU	3.6
1	B	538	LYS	3.6
1	A	150	GLY	3.6
1	B	321	LEU	3.6
1	B	145	TYR	3.6
1	A	136	LEU	3.5
1	C	145	TYR	3.5
1	A	139	LEU	3.4
1	A	537	ALA	3.4
1	B	323	LEU	3.4
1	B	144	PHE	3.3
1	C	538	LYS	3.3
1	A	546	GLY	3.2
1	D	191	ASP	3.2
1	A	137	PRO	3.2
1	D	145	TYR	3.2
1	B	546	GLY	3.2
1	D	192	GLY	3.2
1	C	323	LEU	3.2
1	A	145	TYR	3.2
1	D	194	MET	3.2
1	A	199	LEU	3.1
1	C	186	LEU	3.0
1	A	184	LEU	3.0
1	A	152	GLU	3.0
1	A	195	LEU	3.0
1	B	194	MET	2.9
1	D	195	LEU	2.9
1	D	540	LEU	2.9
1	A	144	PHE	2.9
1	A	194	MET	2.9
1	D	189	THR	2.9
1	C	195	LEU	2.8
1	B	147	ILE	2.8
1	C	314	SER	2.8
1	B	242	SER	2.8
1	C	137	PRO	2.8
1	B	200	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	138	SER	2.8
1	D	190	SER	2.8
1	A	185	THR	2.8
1	B	139	LEU	2.8
1	C	200	PHE	2.7
1	D	199	LEU	2.7
1	D	545	GLU	2.7
1	D	151	GLN	2.7
1	A	147	ILE	2.6
1	A	200	PHE	2.6
1	C	142	LEU	2.6
1	D	184	LEU	2.6
1	B	537	ALA	2.6
1	D	185	THR	2.6
1	D	139	LEU	2.6
1	D	150	GLY	2.6
1	D	147	ILE	2.5
1	B	186	LEU	2.5
1	D	200	PHE	2.5
1	B	148	ALA	2.5
1	C	139	LEU	2.5
1	D	539	LYS	2.5
1	D	152	GLU	2.4
1	B	536	PHE	2.4
1	D	314	SER	2.4
1	C	187	GLN	2.4
1	A	186	LEU	2.4
1	B	187	GLN	2.4
1	C	184	LEU	2.4
1	A	216	ARG	2.4
1	C	144	PHE	2.4
1	D	142	LEU	2.4
1	B	240	LYS	2.4
1	B	185	THR	2.3
1	B	143	LEU	2.3
1	C	151	GLN	2.3
1	B	146	THR	2.3
1	A	544	ARG	2.3
1	B	142	LEU	2.3
1	A	255	LYS	2.3
1	B	314	SER	2.3
1	A	399	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	255	LYS	2.3
1	C	156	VAL	2.3
1	D	186	LEU	2.2
1	B	153	LYS	2.2
1	D	323	LEU	2.1
1	B	403	GLU	2.1
1	B	507	LYS	2.1
1	C	197	LYS	2.1
1	C	194	MET	2.1
1	D	143	LEU	2.1
1	A	247	ALA	2.1
1	C	523	SER	2.1
1	B	545	GLU	2.1
1	A	202	LYS	2.1
1	A	538	LYS	2.1
1	D	507	LYS	2.1
1	C	243	GLY	2.0
1	C	185	THR	2.0
1	B	249	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLU	C	800	10/10	0.81	0.14	48,64,66,66	0
2	GLU	D	800	10/10	0.81	0.18	61,69,70,71	0
2	GLU	A	800	10/10	0.83	0.16	60,63,64,64	0
2	GLU	B	800	10/10	0.84	0.13	49,60,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.